Dimerization of Ethylene by Nickel Phosphino Borate Complexes

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Supporting information

Table S1. The ratio of butenes and hexenes after 1 h of ethylene oligomeration by Method 2[a]

Complex	Butenes[b]	Hexenes
2	74%[c]	26%
3	~100%	-
4	64%	36%

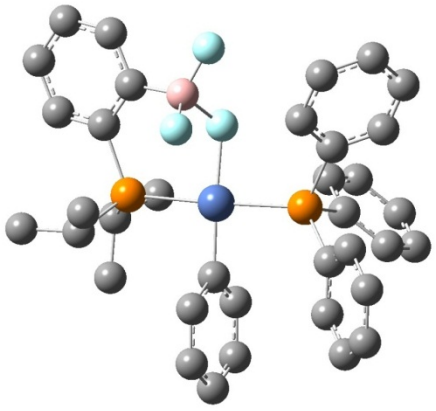
a. Based on GC-MS results (GC[Agilent 6890], column[Agilent HP-5MS], MS[Agilent 5975]: oven temperature from 30°C to 40°C in 1 min, initial time 4 min, run time 5 min). b. 95+% 1-butene. c. These ratios reflect the ratio of butenes to hexenes; small amounts of higher oligomers were also detected by GC-MS at higher oven temperatures, but accurate ratios of all the oligomers were not obtained.

Table S2. Crystallographic Data and Collection Parameters.

	2	**2•NCCH$_3$**	**3**
formula	$C_{36}H_{38}BF_3NiNP_2$	$C_{47}H_{52}BF_3N_2NiP_2$	$C_{25}H_{32}BF_3NNiP$
formula weight	659.12	833.37	504.01
crystal morphology	Orange prism	Yellow needle	Orange prism
dimensions/mm	0.14 x 0.12 x 0.10	0.16 x 0.08 x 0.06	0.18 x 0.16 x 0.12
crystal system	Orthorhombic	Monoclinic	Monoclinic
space group	*P*bca	$P2_1/c$	$P2_1/c$
a/Å	18.8585(3)	8.8931(2)	9.2957(2)
b/Å	16.0547(3)	27.1346(7)	15.6947(5)
c/Å	20.9696(4)	18.1564(5)	16.8650(5)
α/deg	90	90	90
β/deg	90	96.0443(2)	90.285(2)
γ/deg	90	90	90
V, Å^3	6348.9(2)	4356.98(19)	2460.46(12)
Z	8	4	4
d(calc)/mg.m^3	1.379	1.270	1.361
μ(Mo-Kα)/mm^{-1}	0.755	0.566	0.889
T/K	173(2)	173(2)	173(2)
F(000)	2752	1752	1056
total reflections	13824	18221	10216
ind. Reflections	7264	9589	5611
R_1 [$I > 2\sigma(I)$]	0.0527	0.0600	0.0482
wR_2	0.1086	0.1228	0.1040
data/restraints/params	7264/0/392	9589/0/509	5611/0/295
goodness of fit	1.053	1.122	1.084
largest peak/hole e.Å^{-3}	0.436, -0.343	0.360, -0.332	0.435, -0.392

Quantum Chemical Calculations

All geometry optimizations were carried out using the density functional theory with the Gaussian 09 (Revision C.01) program package.[1] The B3LYP functional[2] with Lanl2dz basis set[3] was applied. NBO[4] charges were calculated.



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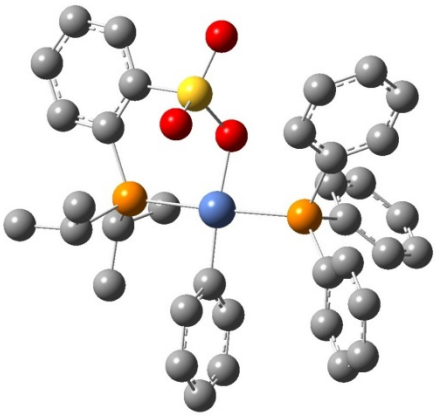

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